Abstract No. crof512

XAS Studies of the Double Perovskites $Ba_{2-x}Sr_xMnReO_6$ System

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Beamline(s): X19A, X18B

Double perovskite, $A_2B'B''O_6$, have been of recent interest for their magnetoresistance properties. Doping of the A site, to increase the perovskite structure tolerance factor, has been shown to enhance the important room temperature low field such materials Our studies of the $Ba_{2-x}Sr_xMnReO_6$ system addressed the magneto-transport response to the tolerance factors variation from 1.0183 (x= 0) to 0.9609 (x= 1). We have also undertaken Mn-K and Re-$L_{2,3}$ edge measurements to firmly establish the important Mn^{2+}-d^5/Re^{6+}-d^1 character of this system. Figure 1 shows the Mn-K edges of A_2ReMnO_6 (A=Ba and Sr), along with the $Mn^{2+}O$ and $LaMn^{3+}O_3$ standards. The proximity of the main edge near μ = 1.0 (see box) and the prominent A-feature at edge-onset with a Mn^{2+} assignment. The prominent B-feature peak at the edge involves 4p final states and it is worth noting that the A=Sr material manifests a distinctly simpler, more intense 4p-feature, compared to the distinctly split 4p feature or the A=Ba spectrum.

The $L_{2,3}$ edges of transition metals exhibit very intense "white line" (WL) features due to transitions into final d-states. For low-d-count perovskite compounds, the octahedral crystal field splitting of the d-states can be observed as a splitting of the WL feature into A/B features related respectively to t_{2g} /e_g final states. Accordingly the relative A to B feature intensity can be used as a probe of the d-occupancy, with increasing A-feature intensity correlating with decreasing d-occupancy. The bimodal A/B WL-features of the Re-L_3 edges, for the double perovskite compounds, are clear in Figure 2. The broadening of the A-B features of the A=Sr compound is presumably due to stronger hybridization effects accompanying the lattice compression. In Figure 3 we show the Ta-$L_{2,3}$ edges for a distorted octahedral Ta^{5+}:d^0 compound $TaNd_{1.4}Ce_{0.6}Sr_2Cu_2O_{10}$. Comparing the Ta-$d^0$ -L_3 spectrum, to the Re-L_3 spectra it is clear that the A-feature is consistently less intense in the Re compounds, corresponding to a Re^{6+},d^1 state. Thus the Mn and Re XAS measurements support the 2+:6+, B:B' character for the B:B' sites in this double perovskite.